

On the Number of Minimal Separators in Graphs

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Abstract. We consider the largest number of minimal separators a graph on n vertices can have at most.

- We give a new proof that this number is in $O\left(\left(\frac{1+\sqrt{5}}{2}\right)^n \cdot n\right)$.
- We prove that this number is in $\omega(1.4521^n)$, improving on the previous best lower bound of $\Omega(3^{n/3}) \subseteq \omega(1.4422^n)$.

This gives also an improved lower bound on the number of potential maximal cliques in a graph. We would like to emphasize that our proofs are short, simple, and elementary.

1 Introduction

For a graph $G = (V, E)$, and two vertices $a, b \in V$, a vertex subset $S \subseteq V \setminus \{a, b\}$ is an (a, b) -separator if a and b are in different connected components of $G - S$, the graph obtained from G by removing the vertices in S . An (a, b) -separator is *minimal* if it does not contain another (a, b) -separator as a subset. A vertex subset $S \subset V$ is a *minimal separator* in G if it is a minimal (a, b) -separator for some pair of distinct vertices $a, b \in V$.

By $\text{sep}(G)$, we denote the number of minimal separators in the graph G . By $\text{sep}(n)$, we denote the maximum number of minimal separators, taken over all graphs on n vertices.

Potential maximal cliques are closely related to minimal separators, especially in the context of chordal graphs. A graph is *chordal* if every induced cycle has length 3. A *triangulation* of a graph G is a chordal supergraph of G obtained by adding edges. A graph H is a *minimal triangulation* of G if it is a triangulation of G and G has no other triangulation that is a subgraph of H . A vertex set is a *potential maximal clique* in G if it is a maximal clique in at least one minimal triangulation of G .

By $\text{pmc}(G)$, we denote the number of potential maximal cliques in the graph G . By $\text{pmc}(n)$, we denote the maximum number of potential maximal cliques, taken over all graphs on n vertices.

Minimal separators and potential maximal cliques have been studied extensively [1,2,3,10,12,15,16,19,20,21]. Upper bounds on $\text{sep}(n)$ are used to upper bound the running time of algorithms for enumerating all minimal separators [1,16,20]. Bounds on both $\text{sep}(n)$ and $\text{pmc}(n)$ are used in analyses of

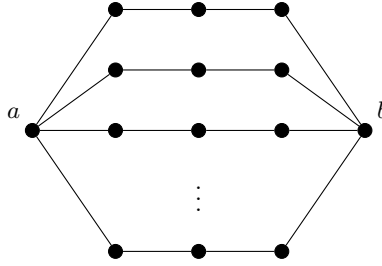


Fig. 1. Melon graphs have $\Omega(3^{n/3})$ minimal separators.

algorithmic running times for computing the treewidth and minimum fill-in of a graph [3,10,12], and for computing a maximum induced subgraph isomorphic to a graph from a family of bounded treewidth graphs [11].

Our results. Fomin et al. [10] proved that $\text{sep}(n) \in O(1.7087^n)$. Fomin and Villanger [12] improved the upper bound and showed that $\text{sep}(n) \in O(\rho^n \cdot n)$, where $\rho = \frac{1+\sqrt{5}}{2} = 1.6180\dots$ ³. We prove the same upper bound with simpler arguments.

As for lower bounds, it is known [10] that $\text{sep}(n) \in \Omega(3^{n/3})$; see Fig. 1. We improve on this lower bound by giving an infinite family of graphs with $\omega(1.4521^n)$ minimal separators. This answers an open question raised numerous times (see, e.g., [9,10]), for example by Fomin and Kratsch [9, page 100], who state

It is an open question, whether the number of minimal separators in every n -vertex graph is $O^*(3^{n/3})$.

Here, the O^* -notation is similar to the O -notation, but hides polynomial factors.

As a corollary, we have that there is an infinite family of graphs, all with $\omega(1.4521^n)$ potential maximal cliques. This answers another open question on lower bounds for potential maximal cliques. For example, Fomin and Villanger [11] state

There are graphs with roughly $3^{n/3} \approx 1.442^n$ potential maximal cliques [10]. Let us remind that by the classical result of Moon and Moser [18] (see also Miller and Muller [17]) that the number of maximal cliques in a graph on n vertices is at most $3^{n/3}$. Can it be that the right upper bound on the number of potential maximal cliques is also roughly $3^{n/3}$? By Theorem 3.2, this would yield a dramatic improvement for many moderate exponential algorithms.

³ The bound stated in [12] is $O(1.6181^n)$, but this stronger bound can be derived from their proof.

Preliminaries. We use standard graph notation from [4]. For an edge uv in a graph G , we denote by G/uv the graph obtained from G by contracting the edge uv , i.e., making u adjacent to $N_G(\{u, v\})$ and removing v .

2 Upper bound on the number of minimal separators

Measure and Conquer is a technique developed for the analysis of exponential time algorithms [7]. Its main idea is to assign a cleverly chosen (sometimes, by solving mathematical programs [5,13,14]) potential function to the instance – a so-called *measure* – to track several features of an instance in solving it. While developed in the realm of exponential-time algorithms, it has also been used to upper bound the number of extremal vertex sets in graphs (see, e.g., [6,8]).

Our new proof upper bounding $\text{sep}(n)$ uses a measure that takes into account the number of vertices of the graph and the difference in size between the separated components of the graph. This simple trick allows us to avoid several complications from [12], including the use of an auxiliary lemma (Lemma 3.1 in [12]), fixing the size of the separators, the discussion of “full components”, and distinguishing between separators of size at most $n/3$ and at least $n/3$.

Theorem 1. $\text{sep}(n) = O(\rho^n \cdot n)$, where $\rho = \frac{1+\sqrt{5}}{2} = 1.6180\dots$ is the golden ratio.

Proof. Let $G = (V, E)$ be any graph on n vertices with $a \in V$. For $d \leq |V|$, an $[a, d]$ -separation is a partition (A, S, B) of V such that

- $a \in A$,
- $G[A]$ is connected,
- S is a minimal (a, b) -separator for some $b \in B$, and
- $|A| \leq |B| - d$.

Let $\text{sep}_a(G, d)$ denote the number of $[a, d]$ -separations in G . By symmetry, $\text{sep}_a(G, 0)$ upper bounds the number of minimal separators in G up to a factor $O(|V|)$. To upper bound $\text{sep}_a(G, d)$, we will use the measure

$$\mu(G, d) = |V| - d.$$

The theorem will follow from the claim that $\text{sep}_a(G, d) \leq \rho^{\mu(G, d)}$ for $0 \leq d \leq |V|$.

If $\mu(G, d) = 0$, then $d = |V|$ and $\text{sep}_a(G, d) = 0$ since there is no $A \subseteq V$ with $|A| \leq 0$ and $a \in A$. If $d_G(a) = 0$, then there is at most one $[a, d]$ -separation, which is $(\{a\}, \emptyset, V \setminus \{a\})$. Therefore, assume $\mu(G, d) \geq 1$, a has at least one neighbor, and assume the claim holds for smaller measures. Consider a vertex $u \in N(a)$. For every $[a, d]$ -separation (A, S, B) , either $u \in S$ or $u \in A$. Therefore, we can upper bound the $[a, d]$ -separations (A, S, B) counted in $\text{sep}_{a,b}(G, d)$ with $u \in S$ by $\rho^{\mu(G-\{u\}, d)} = \rho^{\mu(G, d)-1}$, and those with $u \notin S$ by $\rho^{\mu(G/au, d+1)} = \rho^{\mu(G, d)-2}$. It remains to observe that $\rho^{\mu(G, d)-1} + \rho^{\mu(G, d)-2} = \rho^{\mu(G, d)}$. \square

3 Lower bound on the maximum number of minimal separators

In the melon graph in Fig. 1, each horizontal layer implies a choice between 3 vertices. Each of those choices also ‘costs’ 3 vertices. The new construction improves the bound by adding a vertical choice on top of the horizontal choice. This is achieved by ‘sacrificing’ one of the horizontal choices. This allows us to choose which layer to sacrifice, at the cost of 6 vertices. If it has more than $3 \cdot 3 = 9$ layers, then this will give a larger range of choices than if we hadn’t eliminated that layer.

Theorem 2. $\text{sep}(n) \in \omega(1.4521^n)$.

Proof. We prove the theorem by exhibiting a family of graphs $\{G_1, G_2, \dots\}$ and lower bounding their number of minimal separators.

Let $I = \{1, \dots, 6\}$ and $J = \{1, \dots, 24\}$. The graph G_1 is constructed as follows (see Fig. 2). It has vertex set $V = \{a, b\} \cup \{v_{i,j} : i \in I, j \in J\}$. We denote by V_i the vertex set $\{v_{i,j} : j \in J\}$. The edge set E of G_1 is obtained by first adding the paths $(a, v_{1,j}, v_{2,j}, v_{3,j})$ and $(v_{4,j}, v_{5,j}, v_{6,j}, b)$ for all $j \in J$, and then adding the edges $\{v_{3,j}v_{4,k} : j, k \in J \text{ and } j \neq k\}$. The graph G_ℓ , $\ell \geq 2$, is obtained from ℓ disjoint copies of G_1 , merging the copies of a , and merging the copies of b .

Let us now lower bound the minimal (a, b) -separators \mathcal{S}_j in G_1 that do not contain any vertex from $\{v_{1,j}, v_{2,j}, v_{3,j}, v_{4,j}, v_{5,j}, v_{6,j}\}$ for some $j \in J$. Each such separator contains a vertex from $\{v_{1,k}, v_{2,k}, v_{3,k}\}$, for $k \in J \setminus \{j\}$, since $(a, v_{1,k}, v_{2,k}, v_{3,k}, v_{4,j}, v_{5,j}, v_{6,j}, b)$ is a path in G_1 , and it contains a vertex from $\{v_{4,k}, v_{5,k}, v_{6,k}\}$, for $k \in J \setminus \{j\}$, since $(a, v_{1,j}, v_{2,j}, v_{3,j}, v_{4,k}, v_{5,k}, v_{6,k}, b)$ is a path in G_1 . Due to minimality, the separators in \mathcal{S}_j contain no other vertices. Thus, we have that $|\mathcal{S}_j| = 3^{2 \cdot (|J|-1)}$. We also note that $\mathcal{S}_j \cap \mathcal{S}_k = \emptyset$ if $j \neq k$. Therefore, the number of minimal separators of G_1 is at least⁴ $|J| \cdot 3^{2 \cdot (|J|-1)} > 2.1271 \cdot 10^{23}$.

Minimal (a, b) -separators for G_ℓ are obtained by taking the union of minimal separators for the different copies of G_1 . Their number is therefore at least $(|J| \cdot 3^{2 \cdot (|J|-1)})^\ell = (|J| \cdot 3^{2 \cdot (|J|-1)})^{\frac{n-2}{6 \cdot |J|}} \in \omega(1.4521^n)$, where $n = \ell \cdot 6 \cdot |J| + 2$ is the number of vertices of G_ℓ . \square

Based on results from [2], Bouchitté and Todinca [3] observed that the number of potential maximal cliques in a graph is at least the number of minimal separators divided by the number of vertices n . Therefore, we arrive at the following corollary of Theorem 2.

Corollary 1. $\text{pmc}(n) \in \omega(1.4521^n)$.

⁴ There are also minimal (a, b) -separators that are completely contained in $V_1 \cup V_2 \cup V_3$ or $V_4 \cup V_5 \cup V_6$, but their number does not affect our bound in the first 10 decimal digits in the base of the exponent.

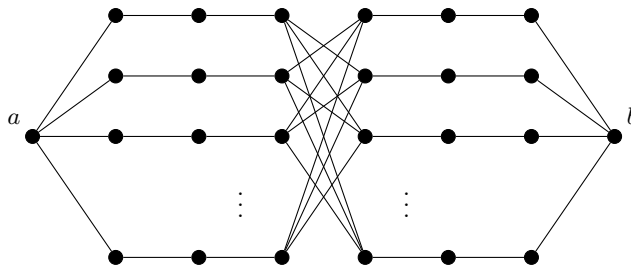


Fig. 2. The graph G_1 has 24 horizontal layers; only 4 are depicted.

4 Conclusion

We have given a simpler proof for the best known asymptotic upper bound on $\text{sep}(n)$, and we have improved the best known lower bound from $\Omega(3^{n/3})$ to $\omega(1.4521^n)$, thereby reducing the gap between the current best lower and upper bound. Before our work, it seemed reasonable to believe that $\text{sep}(n)$ could be asymptotically equal to the best known lower bound. We showed that this is not the case, and we believe there is room to further improve the lower bound.

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